

# **Session 14: Adjoint-Based Design Optimization**

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# Learning Goals

- Introduction and basic approach taken in FUN3D
- Some lingo/nomenclature
- What is an adjoint, and what is it used for?
  - Error estimation and mesh adaptation
  - Sensitivity analysis for design optimization
- Design variables
- Objective/constraint functions
- Geometry parameterizations
- Setup and execution of a simple unconstrained problem
- Things to watch out for
- How to interpret results

What we will *not* cover

- Multipoint/multiobjective/constrained optimization
- Hooking in your own optimizer, parameterization tools
- Forward-mode differentiation using complex variables
- Design of unsteady flows
  - Extremely expensive; know the basics backwards and forwards, then get in touch if still seriously interested



# What to Expect

- Cost of design optimization is very problem-dependent, but in general you can expect to spend ~10 times the cost of a flow solution to get reasonable improvements, depending on how “good” the baseline is
- Generally see very rapid improvements initially, followed by diminishing returns
- We will cover the bare essentials here; also see the website
  - There are many aspects we will not have time to cover here
- This is very much an active research field – be patient, send in questions, and we’ll try to help you through
  - There are a lot of key pieces involved, and getting things running smoothly always involves stumbling blocks along the way



# Design Optimization Using FUN3D

- Based on a gradient-based approach
- FUN3D is distributed with support for several COTS gradient-based optimization packages
  - You must download and install your choice of these third-party libraries
    - PORT (Bell Labs)
    - NPSOL (Stanford)
    - KSOPT (Greg Wrenn)
    - Other packages are generally straightforward to hook up – couple of hours
- These optimizers are based on the user supplying functions and gradients (and perhaps constraints and their gradients also)
  - Optimizers know nothing about CFD, all they see are  $f$  and  $\nabla f$
- In CFD, objective/constraint functions are generally based on things like lift, drag, pitching moment, etc.
  - But can be anything you code up, generally speaking



# Design Optimization Components

## Functions

- When the optimizer requests a function value, it requires a flow solution with inputs and a grid corresponding to the current design variables

## Gradients

- When the optimizer requests a gradient value, it requires a sensitivity analysis with inputs and a grid corresponding to the current design variables
  - The most straightforward way to generate sensitivity information is to perturb each design variable independently and run black-box finite differences
    - This is prohibitively expensive when each finite difference requires a new CFD simulation (or two) – cost scales linearly with the number of design variables!
  - The most efficient sensitivity analysis approach for CFD simulations based on large numbers of design variables (hundreds or thousands) is the adjoint method



# Notation and Governing Equations

We wish to perform rigorous adaptation and design optimization based on the Euler and Navier-Stokes equations, *without requiring any a priori knowledge of the problem:*

$$\frac{\partial \mathbf{Q}}{\partial t} + \mathbf{R}(\mathbf{D}, \mathbf{Q}, \mathbf{X}) = 0$$

$\mathbf{R}$  = Spatial residual

$\mathbf{Q}$  = Dependent variables

$\mathbf{D}$  = Design variables

$\mathbf{X}$  = Computational grid

- Incompressible through hypersonic flows
- May include turbulence models and various physical models from perfect gas through thermochemical nonequilibrium



# What is an Adjoint?

Combine cost function with Lagrange multipliers  $\Lambda$ :

$$L(\mathbf{D}, \mathbf{Q}, \mathbf{X}, \Lambda_f, \Lambda_g) = \underbrace{f(\mathbf{D}, \mathbf{Q}, \mathbf{X})}_{\text{Cost Function}} + \underbrace{\Lambda_f^T \mathbf{R}(\mathbf{D}, \mathbf{Q}, \mathbf{X})}_{\text{Flowfield Equations}} + \underbrace{\Lambda_g^T (\mathbf{K}\mathbf{X} - \mathbf{X}_{surf})}_{\text{Mesh Movement Equations}}$$

$f$  = Cost function (lift/drag/boom/etc)

$\Lambda_f$  = Flowfield adjoint variable

$\mathbf{K}$  = Mesh movement elasticity matrix

$\Lambda_g$  = Grid adjoint variable

Differentiate with respect to  $\mathbf{D}$ :

$$\begin{aligned} \frac{dL}{d\mathbf{D}} = & \frac{\partial f}{\partial \mathbf{D}} + \left[ \frac{\partial \mathbf{R}}{\partial \mathbf{D}} \right]^T \Lambda_f + \left[ \frac{\partial \mathbf{Q}}{\partial \mathbf{D}} \right]^T \left\{ \frac{\partial f}{\partial \mathbf{Q}} + \left[ \frac{\partial \mathbf{R}}{\partial \mathbf{Q}} \right]^T \Lambda_f \right\} \\ & + \left[ \frac{\partial \mathbf{X}}{\partial \mathbf{D}} \right]^T \left\{ \frac{\partial f}{\partial \mathbf{X}} + \left[ \frac{\partial \mathbf{R}}{\partial \mathbf{X}} \right]^T \Lambda_f + \Lambda_g^T \mathbf{K} \right\} - \Lambda_g^T \left[ \frac{\partial \mathbf{X}}{\partial \mathbf{D}} \right]_{surf} \end{aligned}$$

$$\longrightarrow \underbrace{\left[ \frac{\partial \mathbf{R}}{\partial \mathbf{Q}} \right]^T}_{\text{Governing Eqns}} \Lambda_f = - \underbrace{\frac{\partial f}{\partial \mathbf{Q}}}_{\text{Engineering Output}}$$

This adjoint equation for the flowfield has powerful implications for:

- Error estimation & mesh adaptation
- Sensitivity analysis



# Adjoint for Error Estimation and Mesh Adaptation

It is apparent that:

$$\Lambda_f \equiv \frac{\partial f}{\partial \mathbf{R}}$$



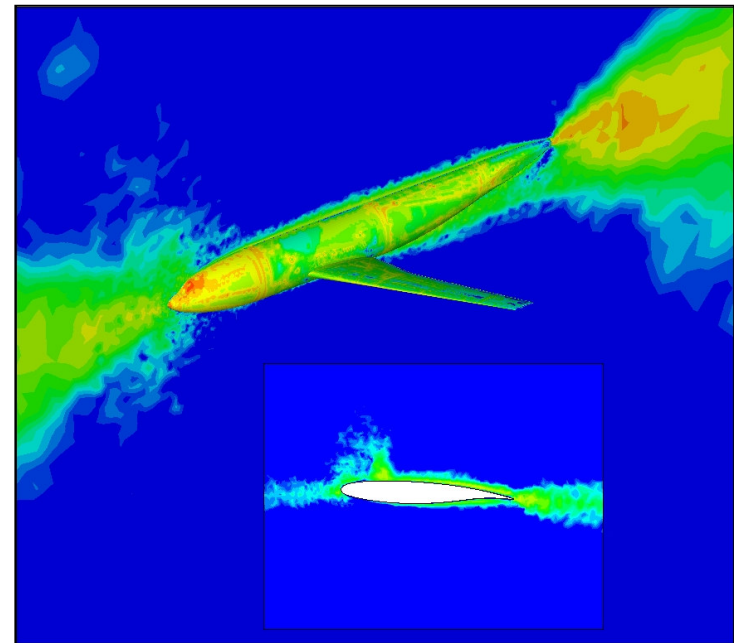
*Direct relationship between local equation error and the output we are interested in!*

- These relationships can be used to get error estimates on  $f$
- Also used to compute a scalar field explicitly relating local point spacing requirements to output accuracy for a user-specified error tolerance
- Often yields non-intuitive insight into gridding requirements
- Relies on underlying mathematics to adapt, rather than heuristics such as solution gradients

User no longer required to be a CFD expert to get the right answer

Transonic Wing-Body:

*“Where do I need to put grid points to get 10 drag counts of accuracy?”*



**Blue=Sufficient Resolution**

**Red=Under-Resolved**

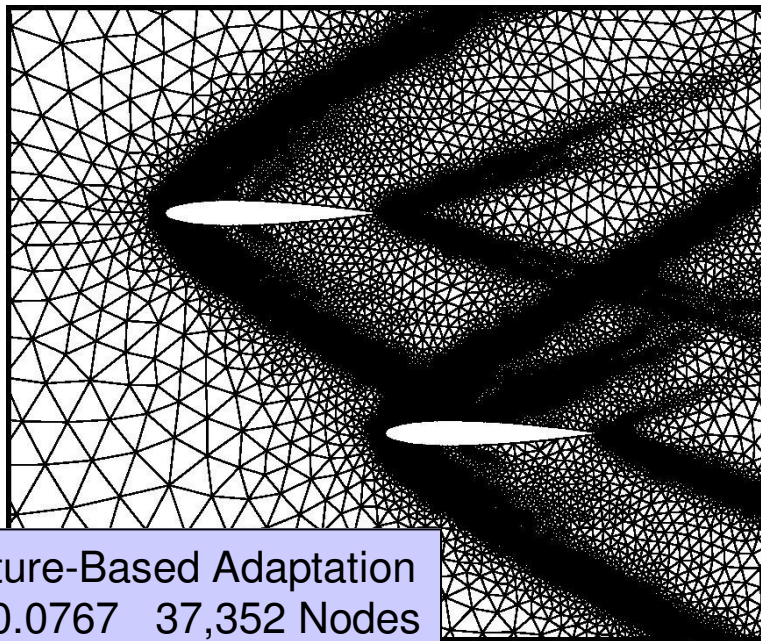
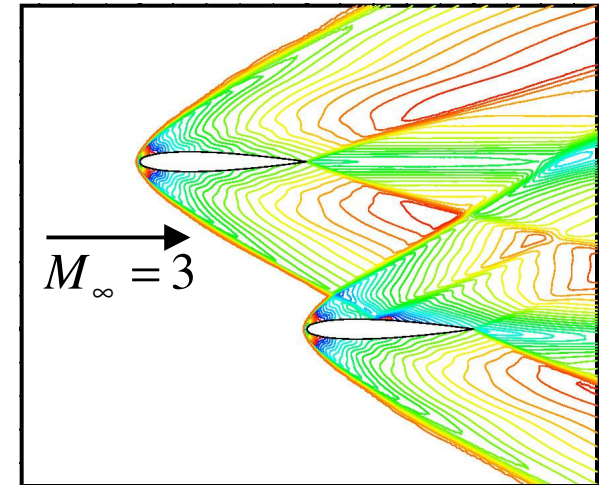




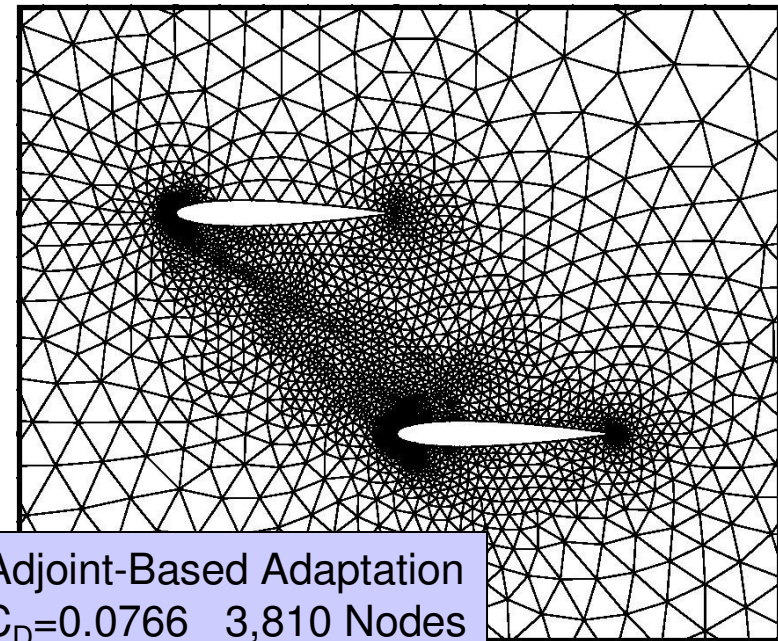
# Supersonic Adjoint-Based Mesh Adaptation

*Collaboration with Venditti/Darmofal of MIT using FUN2D*

- **Objective:** Adapt grid to compute drag on lower airfoil as accurately as possible
- **Result of adjoint-based adaptation:**
  - Uniformly-resolved shocks are not required
  - Drag is computed accurately with a 90% smaller grid



Feature-Based Adaptation  
 $C_D=0.0767$  37,352 Nodes



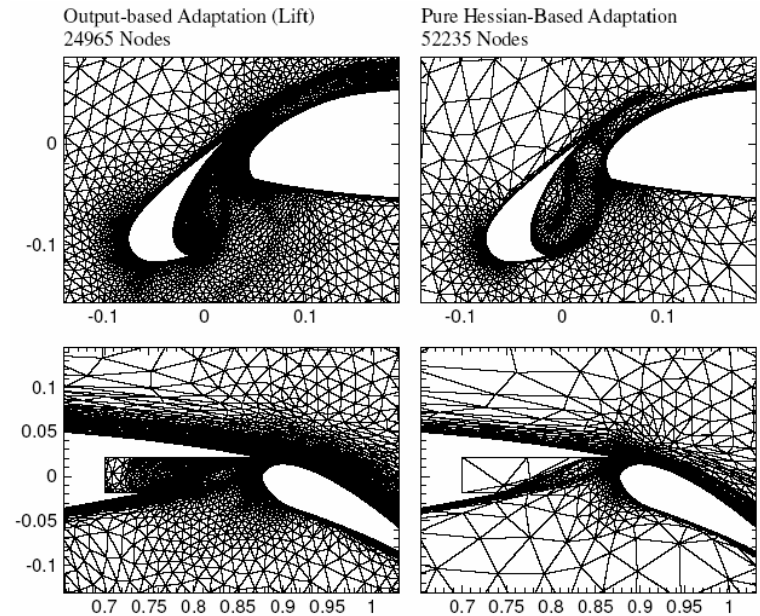
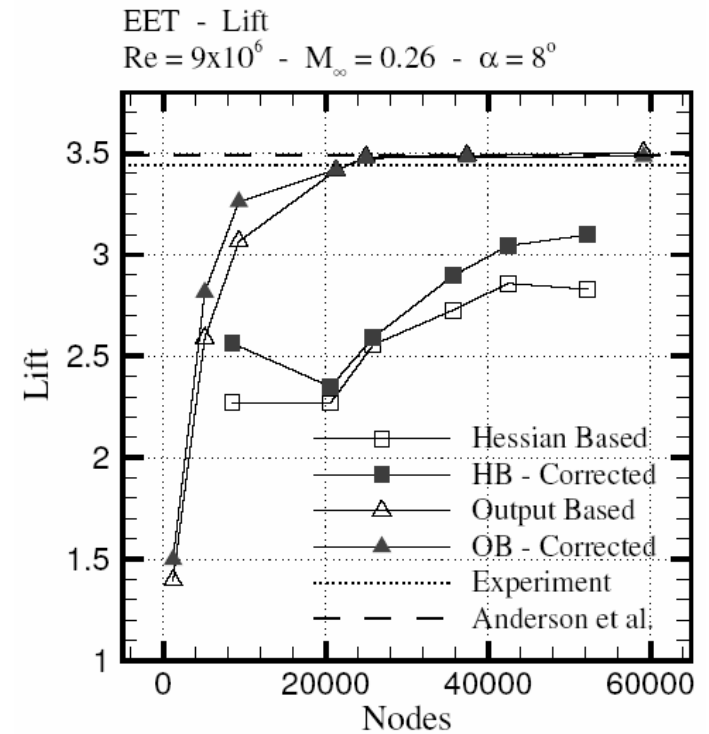
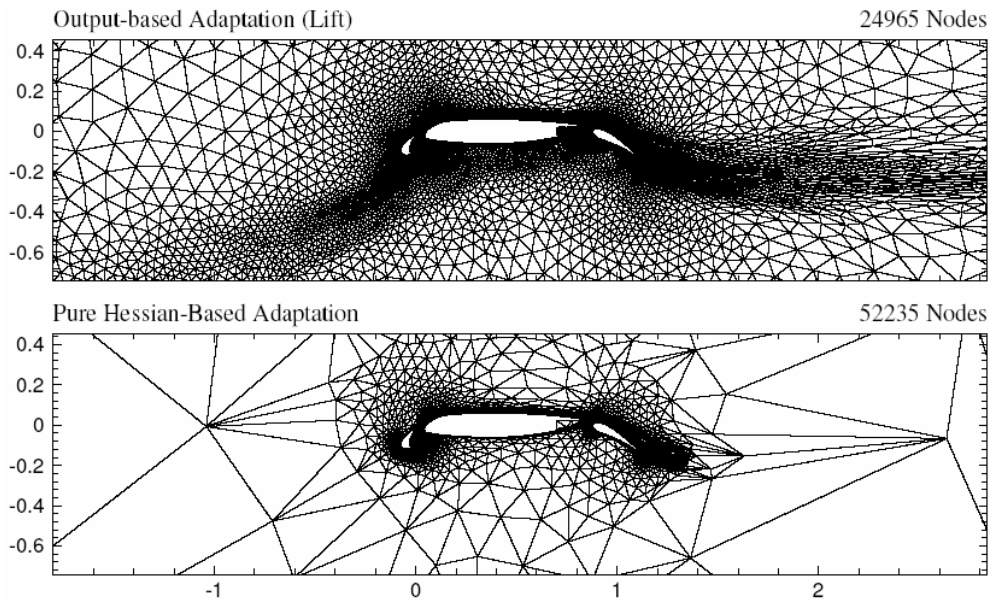
Adjoint-Based Adaptation  
 $C_D=0.0766$  3,810 Nodes



# Adjoint-Based Mesh Adaptation for High Lift

*Collaboration with Venditti/Darmofal of MIT using FUN2D*

- Initial grid was coarse Euler mesh
- Pressure-based indicator only resolves strong flow curvature
- Adjoint-based indicator also includes important smooth regions, stagnation streamline and wakes



# Adjoint for Sensitivity Analysis

Examine the remaining terms in the linearization:

$$\frac{dL}{d\mathbf{D}} = \frac{\partial f}{\partial \mathbf{D}} + \left[ \frac{\partial \mathbf{R}}{\partial \mathbf{D}} \right]^T \Lambda_f + \left[ \frac{\partial \mathbf{X}}{\partial \mathbf{D}} \right]^T \left\{ \frac{\partial f}{\partial \mathbf{X}} + \left[ \frac{\partial \mathbf{R}}{\partial \mathbf{X}} \right]^T \Lambda_f + \Lambda_g^T \mathbf{K} \right\} - \Lambda_g^T \left[ \frac{\partial \mathbf{X}}{\partial \mathbf{D}} \right]_{surf}$$

$$\longrightarrow \mathbf{K}^T \Lambda_g = - \left\{ \frac{\partial f}{\partial \mathbf{X}} + \left[ \frac{\partial \mathbf{R}}{\partial \mathbf{X}} \right]^T \Lambda_f \right\} \quad \text{Discrete adjoint equation for mesh movement}$$

$$\longrightarrow \frac{dL}{d\mathbf{D}} = \frac{\partial f}{\partial \mathbf{D}} + \Lambda_f^T \frac{\partial \mathbf{R}}{\partial \mathbf{D}} - \Lambda_g^T \left[ \frac{\partial \mathbf{X}}{\partial \mathbf{D}} \right]_{surf} \quad \text{Sensitivity equation}$$

## Function Evaluation

1. Compute surface mesh at current  $\mathbf{D}$
2. Solve mesh movement equations
3. Solve flowfield equations

## Sensitivity Evaluation

3. Solve flowfield adjoint equations
2. Solve mesh adjoint equations
1. Matrix-vector product over surface

**Analysis Cost = Sensitivity Analysis Cost**

Even for **1000's** of design variables



# Design Variables in FUN3D

- Global flowfield variables
  - Mach number, angle of attack
- Shape variables
  - These depend entirely on the geometric parameterization being supplied to FUN3D; FUN3D has no native shape variables, other than the grid points themselves
- Additional variables related to unsteady simulations



# Objective/Constraint Functions in FUN3D

$$f_i = \sum_{j=1}^{J_i} \omega_j (C_j - C_j^*)^{p_j}$$

$\omega$  = weight     $C$  = aero coeff  
 $p$  = power     $C^*$  = target aero coeff

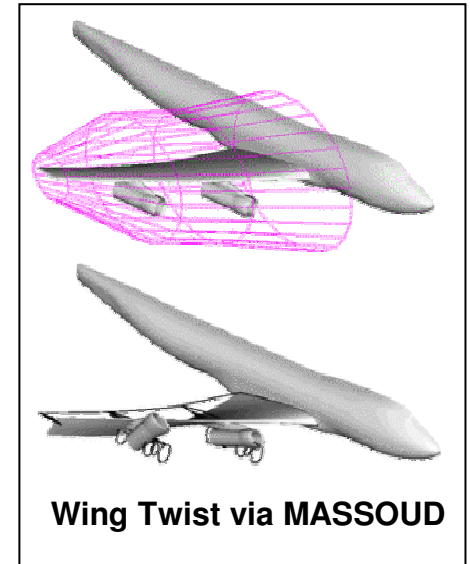
- User may specify which boundary patch in the grid (or all) to which each function applies
- Constraints may be explicit or added as “penalties”
- Multipoint/multiobjective: as many composite functions/constraints as desired
  - Only limited by particular optimization package
  - Adjoints for multiple functions/constraints computed simultaneously
- The optimization always seeks to *minimize* the objective function(s), so pose them accordingly



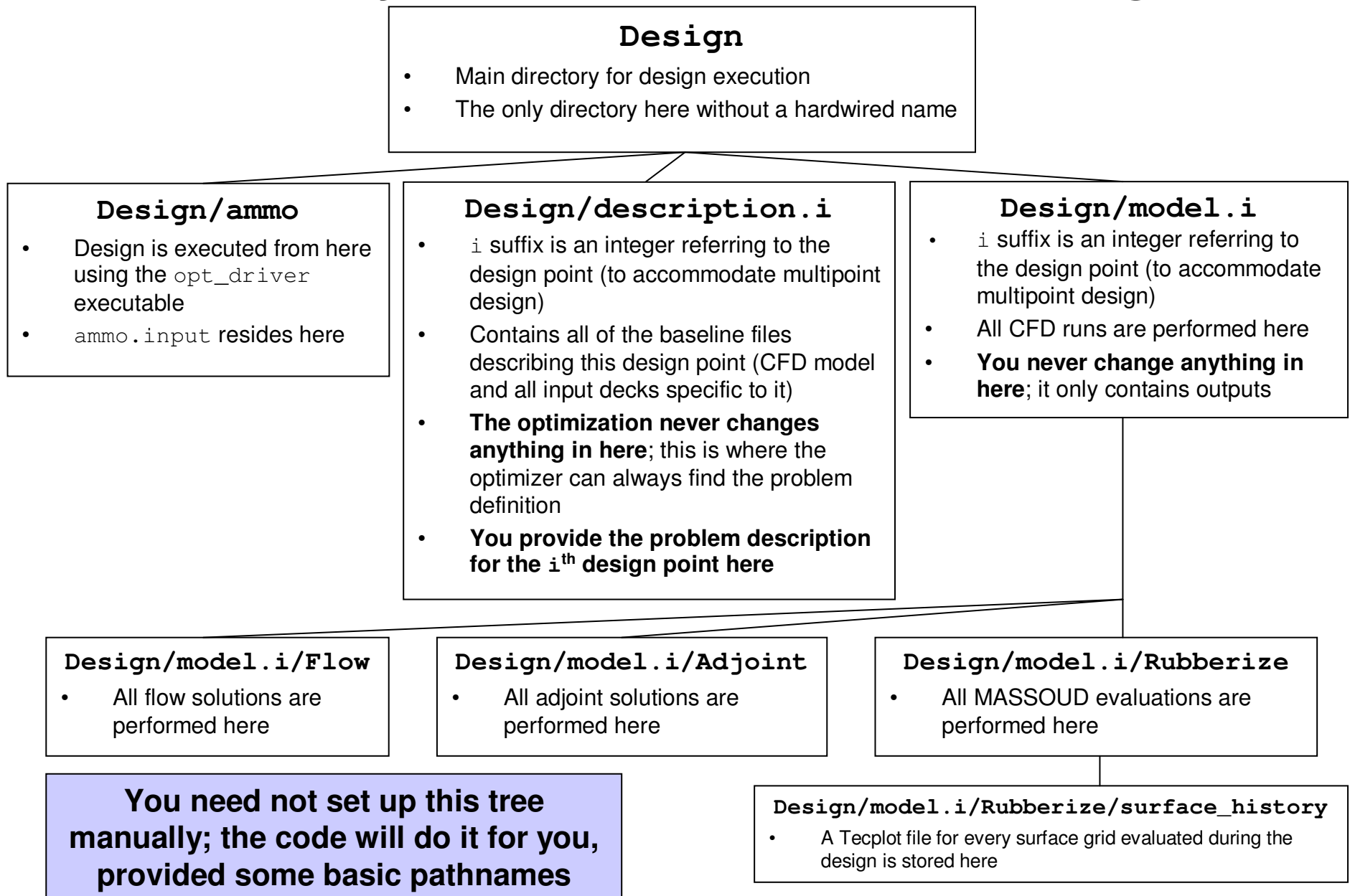


# Geometry Parameterizations

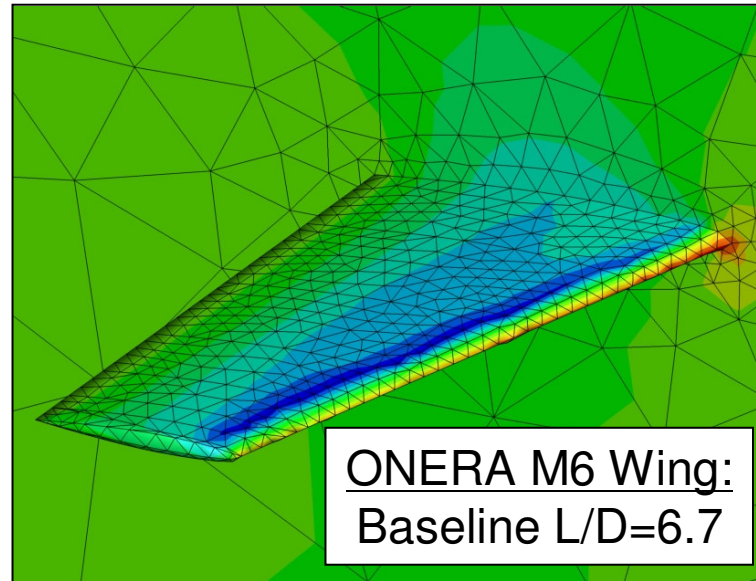
- FUN3D relies on a pre-defined relationship between a set of parameters, or design variables, and the discrete surface mesh coordinates
- Given  $\mathbf{D}$ , surface parameterization determines  $\mathbf{X}_{surf}$  (surface mesh)
- For example, given the current value of wing thickness at a location, what are the corresponding xyz-coordinates of the mesh?
- This narrows down the number of design variables from hundreds of thousands (raw grid points) to dozens or hundreds
  - Optimizers will perform more efficiently
  - Smoother design space
- The other requirement of the parameterization package is that it provides the Jacobian of the relationship between the design variables and the surface mesh,  $\partial\mathbf{X}_{surf}/\partial\mathbf{D}$
- While FUN3D users may provide their own parameterization scheme, most choose to use one of two Langley-provided packages based on free-form deformation algorithms:
  - MASSOUD: Aircraft-centric design variables (thickness, camber, planform, twist, etc)
  - Bandadds: General patching tool to handle fillets, winglets, and other odd shapes
  - Both packages maintained by Jamshid Samareh of NASA LaRC
- To dump out the surface grids in the Tecplot format necessary for these tools, run the flow solver with `'--write_massoud_file'`
  - This procedure generates a `[project]_massoud_bndryN.dat` file for the  $i^{\text{th}}$  solid boundary



# Directory Tree for FUN3D-Based Design



# Demo: Maximize L/D for Transonic Flow Over a Wing



- Log into your account on `cypher-work14`
- Go down into the `Design_Demos` directory  
`'cd Design_Demos'`
- Go down into the `Wing` directory  
`'cd Wing'`
- To build the directory tree we just described, you would normally run  
`'/path/to/your/FUN3D/installation/Design/opt_driver --setup_design 1'`
  - After entering a couple of pathnames, it would build the tree for you





# Demo: Maximize L/D for Transonic Flow Over a Wing

- Do an `'ls'` in your current directory
- You will see the following directory structure:
  - The `ammo` subdirectory contains the high-level inputs for the optimization
    - You will set up one file in here to control the actual optimization
  - The `description.1` directory must contain all of the baseline files related to the first design point (grid, parameterization, solver input deck, etc)
    - This is the primary location you need to fill up with input files ahead of time
    - During the course of the optimization, the codes will always look here for the baseline files related to the first design point
    - The optimization procedure will *never* write to this directory; it is designed to store the problem definition
  - The `model.1` directory contains three subdirectories in which the actual CFD will be performed for the first design point:
    - `Adjoint` is where the adjoint solutions will take place
    - `Flow` is where the flow solutions will take place
    - `Rubberize` is where the parameterizations are evaluated
  - *You do not need to set anything in the `model.1` directories* – they will be populated during the course of the design and only contain outputs



# ***Demo: Maximize L/D for Transonic Flow Over a Wing***

- Go down into the `description.1` directory
- These are the files you would normally have to provide in the `description.i` directory for a typical design – let's walk through and look at each of them...

## **`command_line.options`**

- This file is used to specify any command line options (CLO's) required by each of the FUN3D executables
- The first line specifies the number of executables for which you are providing CLO's
- This is followed by a line containing an integer and a keyword
  - The integer specifies the number of CLO's you are providing for the code identified by the keyword
- This is followed by the actual CLO's for the current executable
- Note 'mpirun' is an available keyword: this provides the opportunity to feed your `mpirun` executable any options it may require (`-nolocal`, `-machinefile filename`, etc.)
  - Depends on your environment, queue structure, etc.



# ***Demo: Maximize L/D for Transonic Flow Over a Wing***

**design.1, design.gp.1**

- These files are input files for MASSOUD for the 1<sup>st</sup> body; the MASSOUD setup tool provides these when you set up your parameterization
- Do not change these files

**design.usd.1**

- This file is an input file for MASSOUD for the 1<sup>st</sup> body; the MASSOUD setup tool provides this template when you set up your parameterization
- Depending on how you choose to “link” raw MASSOUD variables to create new variables, this defines the linking weights (see MASSOUD documentation)
- When using MASSOUD with FUN3D, you must always use the design variable linking option, even if simply set to the identity matrix



# ***Demo: Maximize L/D for Transonic Flow Over a Wing***

## **massoud.1**

- This file tells MASSOUD the names of its input/output files for the 1<sup>st</sup> body
- The first value specifies the number of linked MASSOUD design variables
  - If linking matrix is identity, this is just the number of raw MASSOUD design variables
- The remainder of the inputs are filenames; they should remain as is, but with the integer value in each name set to the index of the current body



# ***Demo: Maximize L/D for Transonic Flow Over a Wing***

## **`fun3d.nml`**

- This is the nominal solver input deck for your case
- The adjoint solver also uses this input
  - If the adjoint requires different values (e.g., stopping tolerance), you can override these values with CLO's given in `command_line.options`
- It should contain the necessary inputs to run the baseline case
- The optimization will override values as needed using CLO's (e.g., angle of attack, etc)

## **`inviscid.fgrid, inviscid.mapbc`**

- This is the nominal mesh for your baseline case
- This particular grid is in FAST format; VGRID format is also allowed
- Note the symmetry plane has been given a 3080 BC index – this is recommended for symmetry planes during design optimization



# ***Demo: Maximize L/D for Transonic Flow Over a Wing***

## **rubber.data**

- This file is used to define the design variables and their bounds, objective functions, and constraints for the current design point
- A copy of this file is placed in the `model.1` directory at the beginning of an optimization and is continuously updated with the current values of the design variables, objective/constraint functions, and all gradient information
  - If you want to know the latest info during a design, it's probably in here



# ***Demo: Maximize L/D for Transonic Flow Over a Wing***

**rubber.data**

## Code Status Block

- Leave alone

## Design Variable Block

- In general, for each design variable, you must set several fields
  - Active (0=no, 1=yes), baseline value, upper and lower bounds (if active)
- First subsection lays out the Mach number and angle-of-attack information
- This is followed by an input stating the number of bodies to be designed
- Then for each body:
  - Fixed number of rigid motion variables – leave these alone
  - Number of shape variables and their inputs – these correspond directly to the MASSOUD variables previously discussed
    - When setting bounds for shape variables, it pays to be conservative – the optimizer will exploit every radical shape it can dream up
    - You can quickly get into unsolve-able or invalid/crossed-up geometries
    - You can always loosen up the bounds and restart the design if needed



# Demo: Maximize L/D for Transonic Flow Over a Wing

`rubber.data`

## Function Block

- These sections lay out the objective/constraint function definitions
- First input is the total number of composite functions being specified (sum of objectives + constraints)
- Then, for each function:
  - Is it an objective function (1) or a constraint (2)
  - If it is a constraint, what are the upper and lower bounds (otherwise dummies)
  - How many component functions are used to build up the composite function
  - Time step interval defining the function (leave as dummies – for unsteady design)
  - Then the list of component functions:
    - Boundary index it applies to (0 means all boundaries)
    - Keyword identifying the function type (see header of LibF90/forces.f90)
    - Value (dummy – this is an output during the optimization)
    - Weight to be applied to current component function
    - Target value for current component function
    - Exponent for current component function
    - The remainder of the function block is devoted to sensitivity outputs – you can place dummies here, *but there must be a line corresponding to every design variable*

Our objective function:

$$f = (L/D - 20)^2$$





# ***Demo: Maximize L/D for Transonic Flow Over a Wing***

- We are now finished setting things up in the `description.1` directory
- Finally, head over to the `../ammo` directory
- There is only a single file here that needs to be set up
  - The `ammo.input` file controls the actual optimization procedure
- Let's walk through this file real quick...

## **`ammo.input`**

- Change USERNAME to your username in the absolute path variable
- Everything else documented on the website, but a few reminders:
  - Optimization packages: `KSOPT=3`, `PORT=4`, `NPSOL=5`
  - Grid types: `FAST=1`, `VGRID=2`
  - Operation to perform: `analysis=1`, `sensitivity analysis=2`, `optimization=3`
  - Note you can specify the `mpirun` executable name
    - Useful if executable is called 'mpixec' or otherwise on your system



# Demo: Maximize L/D for Transonic Flow Over a Wing

*Enough with problem setup, let's do something already!*

- The first thing I typically do is just run a function evaluation to see that the parameterization and all of the inputs are set correctly
- To do this, edit `ammo.input` and set `Operation to Perform to 1`
- The command line that is used to run this case is  
`opt_driver --sleep_delay 5 > screen.output`
  - The '`--sleep_delay 5`' instructs the driver to wait 5 seconds in between operations – allows NFS caching to keep up
- Submit the job using '`qsub qinput`'



# ***Demo: Maximize L/D for Transonic Flow Over a Wing***

- The first thing that you will see is MASSOUD evaluating the parameterization for each body, defining the surface grid coordinates at the baseline position
- The flow solver will then start up, but prior to the solve, you will see an auxiliary solution take place that represents the interior mesh movement based on the elasticity equations
  - For this first step at the baseline position, you should see very small numbers for the “Error Estimate”: this indicates the current mesh is very close to the desired mesh
- After the actual flow solution takes place, the solver will evaluate each of the objective and constraint functions you posed:  

```
Current value of function      1      176.932026370194
```
- This marks the end of a successful function evaluation
- Always wise to plot the flow solver convergence – you want to run enough iterations to get a “reasonable” answer, but you don’t necessarily need to drive it into the ground



# Demo: Maximize L/D for Transonic Flow Over a Wing

- Now lets try a sensitivity analysis
- Edit `ammo.input` and set `Operation` to `Perform to 2`
- Submit the job
- The first thing that will take place is a function evaluation, just as before
- After the function evaluation takes place, MASSOUD will fire up again to evaluate the linearizations of the surface mesh coordinates with respect to the design variables
- FUN3D's adjoint solver will then start up:
  - You will see a solution taking place; this is the flowfield adjoint
  - Afterwards, you will see another solution occurring; this is the elasticity adjoint for the mesh
  - The final step is to update the `model.1/rubber.data` file with the sensitivity information
- This marks the end of a successful sensitivity analysis
- Again, it is wise to plot the convergence of the flowfield adjoint system
  - This convergence history is in the `model.1/Adjoint/inviscid_hist.tec` file
  - In general, you want 2-3 orders of magnitude convergence; this is usually sufficient for reasonable sensitivity information



## Demo: Maximize L/D for Transonic Flow Over a Wing

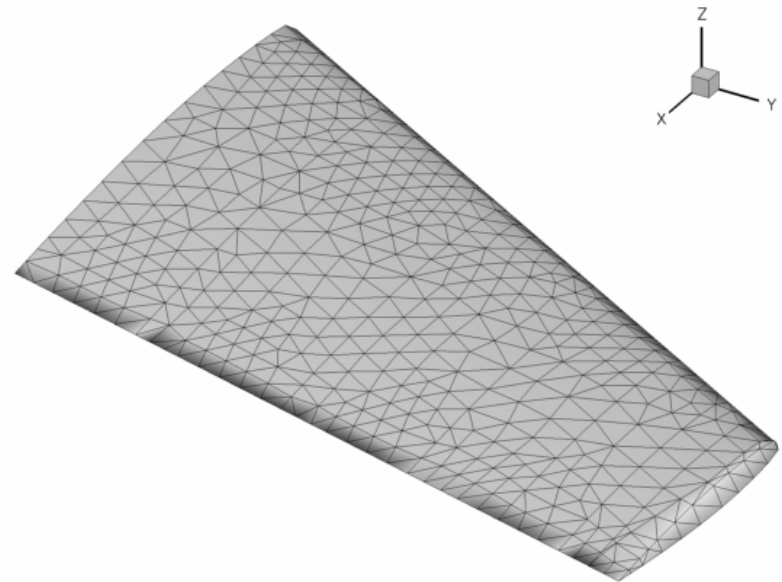
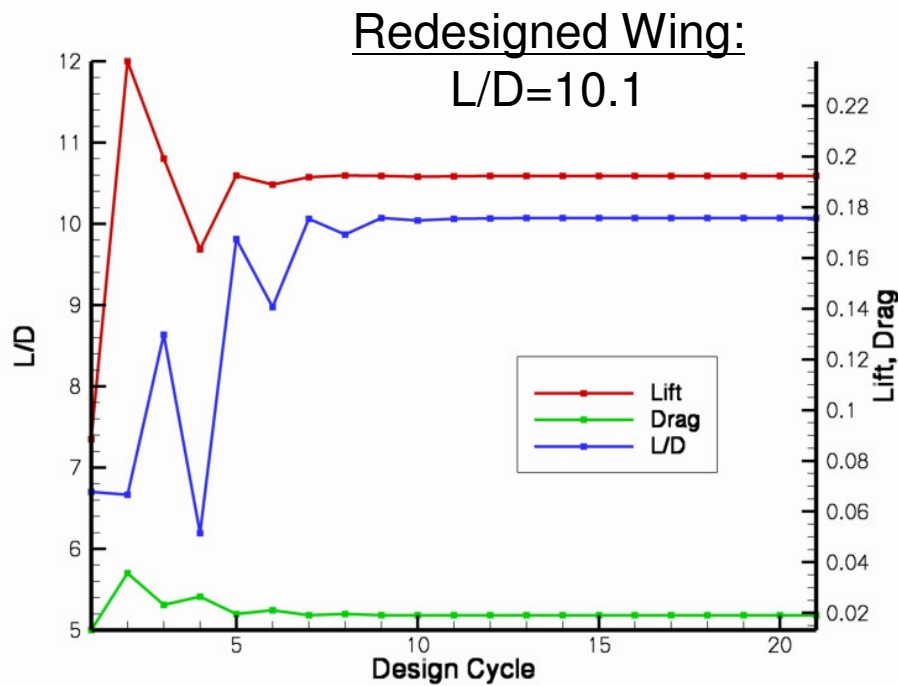
- If you got this far, things are looking pretty good – we’ve checked that everything is set up to run functions and gradients correctly, which is all the optimizer depends on
- Now we’re ready to try an actual optimization
  - Edit `ammo.input` and set `Operation` to `Perform` to 3; submit the job
- Now you will see a lot of function and gradient evaluations going by, as the optimizer starts to change design variables and search for an optimum solution
- One easy way to monitor progress is to:
  - ‘`grep “Current value” screen.output`’:

Current value of function	1	176.932026370194
Current value of function	1	177.821434003674
Current value of function	1	129.220241755776
Current value of function	1	190.673990365144
Current value of function	1	103.748612625773
Current value of function	1	121.518003185828
Current value of function	1	98.7934314688426
Current value of function	1	102.714508670476
Current value of function	1	98.5477600125918
Current value of function	1	99.1776524751379
Current value of function	1	98.7862106497303
- You can also observe (but don’t change!) the file `model.1/rubber.data`



## Demo: Maximize L/D for Transonic Flow Over a Wing

- After the job finishes, PORT will summarize its performance in the file `model.1/port.output`
- Since each solution is a warm start, you can plot the entire flow solution history contained in `model.1/Flow/inviscid_hist.tec`
- A history of the surface geometry is stored in `model.1/Flow/movie.tec`
  - Use Tecplot's animate capability to view the evolution of the geometry/solution



# ***Demo: Maximize L/D for Transonic Flow Over a Wing***

## *What Could Possibly Go Wrong?*

- The procedure can terminate due to CFD-related problems:
  - Running into negative volumes during a mesh movement (you can plot the history of the surface(s) using the files in `model.1/Rubberize/surface_history`)
    - Watch for invalid surfaces or unusually large changes
    - Be conservative in your lower/upper bounds!
  - The flowfield or the adjoint solution is unstable
    - Problem-dependent; get in touch for advice
- The procedure can also terminate due to hardware/environment problems
  - You run out of allocated time, a node dies, etc.
- Finally, the procedure can terminate if the optimizer has given up:
  - No more progress can be made due to constraints
  - The optimizer has hit the max number of functions/gradients you allowed
  - An optimal solution has been found



# List of Key Input/Output Files

- Input
  - All files necessary to run solutions for each design point (grid files, `fun3d.nml`, etc)
  - All MASSOUD files for  $i^{\text{th}}$  parameterized body (`design.i`, `design.usd.i`, `design.gp.i`, `massoud.i`)
  - `command_line.options`
  - `rubber.data`
  - `ammo.input`
- Output
  - All files normally associated with running the solver
  - `rubber.data`
  - `port.output`
  - `movie.tec`





# Summary of FUN3D-Based Design Optimization

- That's more or less the basic pieces involved with running an optimization
- Lots of options we did not cover here; see website or get in touch for help
  - How the wrappers work (`LibF90/analysis.f90`, `LibF90/sensitivity.f90`)
  - Parameterizations other than MASSOUD
  - Multipoint/multiobjective (tutorial on website)
  - Constrained problems (tutorial on website)
  - Running with other optimization packages (tutorial on website)
  - Body grouping, spatial transforms
  - Forward-mode sensitivity analysis using complex variables
  - Unsteady design (*expensive*)

## General Advice

- Become very comfortable with the flow solver
- Work the website tutorials
- Learn how to set up parameterizations using MASSOUD and/or bandaids
- Try plugging in your own grids/parameterizations in the tutorials
- Ask questions – it's actually not that bad once you get up the learning curve



# What We Learned

- General approach used by FUN3D for design optimization
- What is an adjoint
- What does a function/gradient evaluation consist of in terms of CFD
- Design variables in FUN3D
- Functions/constraints in FUN3D
- What is required of a geometry parameterization tool
- How to set up the inputs required for design optimization
- How to run function, gradient evaluations
- How to perform a basic design optimization
- What to watch out for and how to interpret results

*Have fun and don't hesitate to send questions our way!*

***[fun3d-support@lists.nasa.gov](mailto:fun3d-support@lists.nasa.gov)***

